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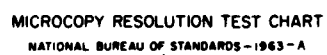
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SIXTH INTERNATIONAL SUMMER INSTITUTE IN SURFACE SCIENCE  
(ISISS 1983)

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The academic goals of ISISS were outlined in the editorial comments of "Surface Science: Recent Progress and Perspectives (ISISS 1975)":

"The favorable acceptance of ISISS was gratifying, but did not exactly come as a surprise. During the recent decade, advanced ultrahigh vacuum technology has made the achievement of pressures  $< 10^{-10}$  Torr a routine operation so that surfaces, once freed from impurities, can be kept clean over a sufficient length of time and adsorbates then can be admitted at well-dosed amounts. Techniques for surface analysis were more and more refined; with the atom probe we are now able to analyze even single surface atoms or chemical complexes. Progress in the theory of the solid state subsequently allowed some fruitful dealing with the theoretical aspects of solid surfaces. All these developments combined with the demand for data by vital branches of our modern technology, caused an increasing flood of publications especially in the field of gas-solid interfaces. It became hard to catch up with the literature in one's own narrow area and it appeared nearly impossible to keep track of the developments in neighboring fields. As in other fast developing parts of the natural sciences, one consequently observes some isolationism and the appearance of communication problems. It is quite clear that such a tendency, where one no longer learns from progress or setbacks in neighboring areas, would be very much to our disadvantage. To counteract this tendency, ISISS was organized. Leading experts from various subdivisions of surface science - we chose to restrict the topics to gas-solid interfaces - presented tutorial review talks in which recent progress was summarized and future trends were pointed out."

In order to keep ISISS 1983 at a level of highest quality all former ISISS speakers were invited to suggest names of suitable lecturers. To avoid duplication, none of the lecturers of the 1981 Summer Institute were invited to present a paper. The final list showed twenty-one internationally known experts in the field of gas-solid interfaces. The speakers came from Germany, Mexico, New Zealand, South Africa, Switzerland, and from the U.S.A.

The following list shows their names, their affiliations, topics, and short summaries of the papers presented.



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P. Bak, Brookhaven National Laboratory, Upton, New York

### Commensurate-Incommensurate Transitions on Surfaces ;

Layers of atoms or molecules adsorbed on surfaces may exhibit transitions between commensurate and incommensurate ordered structures. Krypton adsorbed on graphite goes from a  $\sqrt{3} \times \sqrt{3}$  phase to an incommensurate phase with hexagonal symmetry, freon on graphite has a transition from a  $2 \times 2$  structure to a uniaxial incommensurate phase, and Xe on Cu{110} and H on Fe{110} undergo transitions between uniaxial commensurate phases and striped incommensurate phases. As the temperature is raised the 2d ordered structures melt into disordered liquid phases.

This lecture reviews recent experimental and theoretical work on phase transitions and phase diagrams of two-dimensional systems with commensurate, incommensurate and fluid phases. According to current theories, the commensurate-incommensurate transition is brought about by spontaneous formation of walls, or solitons; the melting transition is caused by dislocation separation. The structure of the phase diagram is thus determined by the interplay between two types of topological defects, solitons and dislocations. The structure of the phase diagram depends in a crucial way on the order of commensurability and on the symmetry of the various phases. For high order of commensurability floating commensurate phases may exist just below the melting transition, and for low order commensurability the fluid phase may penetrate all the way to zero temperature. The need for further experiments to test specific theoretical predictions on the phase diagrams and the critical behavior near the transitions will be emphasized.

A. T. Bell, University of California, Berkeley, California

### Fourier-Transform Infrared Spectroscopy in Heterogeneous Catalysis

Infrared spectroscopy is one of the most widely used techniques for characterizing the surface structure of heterogeneous catalysts and the structures of adsorbed species. Fourier-transform spectroscopy makes it possible to acquire infrared spectra with good signal-to-noise ratio, in times as short as a few tenths of a second. This makes it possible to characterize materials under dynamic conditions and in steady-state situation where the level of light at the detector is low. This presentation will cover the fundamentals of Fourier-transform spectroscopy and will illustrate how the technique can be used to study a variety of problems. The use of FTS to acquire spectra vs transmission, specular reflectance, diffuse reflectance, and emission methods will also be discussed.

R. Cavanagh, National Bureau of Standards, Washington, D.C.

→ Laser Studies of Surface Chemical Reactions ; 2, 3

I. Lasers and Surface: Overview

- a. Spectroscopy
- b. Speciation
- c. Materials and Device Preparation
- d. Non Linear Optical Phenomena
- e. Chemical Dynamics
- f. Time Domain

II. Chemical Dynamics at Surfaces

- a. Basis in Gas Phase Chemical Dynamics
- b. Inelastic Scattering: Gas Phase Scattering vs.  
Surface Scattering - Example NO/Ag{111}
  - 1. Kinetic Energy Dependence
  - 2. Rainbows
  - 3. Polarization
- c. Reactive Scattering: Gas Phase Reactions vs.  
Surface Reactions - Example NO/Ru{001}
  - 1. Rotational Distribution
  - 2. Doppler Effect
  - 3. Flux Distribution
- d. Impact on Surface Chemistry and Surface Physics

III. Time Domain Measurements

- a. Energy Transfer Measurements in Real Time - Why?
- b. Gas Phase and Liquid Phase measurements
  - 1. Techniques
  - 2. Observations
- c. Surface Experiments
  - 1. Picosecond IR Pump-Probe
  - 2. Visible Fluorescence Rise and Decay Times

IV. Future Directions

- a. Materials Processing
- b. Molecular Dynamics: Recombination
  - ESD
  - PSD
- c. Real Time Measurements

J. D. Dow, University of Notre Dame, Notre Dame, Indiana

Intrinsic and Extrinsic Surface Electronic States of Semiconductors .

In the bulk of a tetrahedral semiconductor, a single substitutional s-p bonded impurity or vacancy will ordinarily produce four "deep" levels with energies near the fundamental band gap: one s-like ( $A_1$ ) and three p-like ( $T_2$ ). These deep levels may lie within the fundamental band gap, in which case they are conventional deep levels, or they may lie within the band as "deep resonances." A sheet of  $N$  vacancies will produce  $4N$  such deep levels -- namely, the surface state energy bands, which may or may not overlap the fundamental gap (to a good approximation, insertion of a sheet of vacancies is equivalent to creating a surface).

Intrinsic surface states have common underlying physics with deep impurities, and so their energies can be relatively easily predicted by extending to surface ideas developed by Hjalmarson, Vogl, Wolford, et al. for the deep impurity problem. This has been done by Allen et al.

The energies of extrinsic surface states also are governed by similar physics, and are especially interesting in the light of the Schottky barrier problem: Bardeen showed that modest densities of surface states on a semiconductor can "pin" the Fermi level, forming a Schottky barrier. The bulk Fermi energies of the semiconductor, the metal, and the semiconductor surface must align. If the semiconductor is heavily doped n-type, the surface Fermi energy is the lowest empty surface state. The bands bend to accommodate this alignment of Fermi levels, forming the Schottky barrier. Thus the Schottky barrier height is the binding energy of the lowest naturally empty surface state, relative to the conduction band edge. Sice et al., have recently proposed that the Bardeen surface states responsible for pinning the Fermi energy are due to native defects. Brillson and co-workers have argued that the barrier height correlates with chemical reactivity of the metal. We believe that both are correct.

Daw, Smith, Swarts, and McGill have proposed that free surfaces vacancies account for some of the observed Schottky barrier heights. Allen and co-workers have argued that antisite defects "sheltered" at the surface pin the Fermi energy for most Schottky barriers between III-V semiconductors and non-reactive metals, but that vacancies become the dominant pinning defect when the metal is reactive. Thus the Brillson reactivity picture can be unified with the Fermi-level pinning picture: the chemical reaction merely changes the dominant pinning defect. The experimental results of Mead and Spitzer, Wieder, Williams, Monch, their co-workers, and many others support this general viewpoint.

Moreover, the connection between the Schottky barriers formed at Si interfaces with transition metal silicides and the barriers between III-V semiconductors and metals appears to be provided by the recent work of Sankey et al.: Fermi-level pinning can account for the silicide data as well. Thus a single unifying picture of Schottky barrier heights in III-V

and homopolar semiconductors appears to be emerging. And although this Fermi-level pinning picture is no doubt oversimplified, it does provide a simple explanation of the first-order physics determining Schottky barrier heights, and how the physics changes when the dominant defect switches as a result of chemical reactivity.

J. A. Dumesic, and B. J. Tatarchuk, Auburn University, Alabama

Mössbauer Spectroscopy: Applications to Surface and Catalytic Phenomena

- I. Brief introduction to the principles of transmission Mössbauer spectroscopy and applications to bulk-type measurements.
- II. Physical principles of conversion electron Mössbauer spectroscopy (CEMS) and collection of "surface-specific" information.
- III. Past experimental efforts using CEMS: equipment and surface information.
- IV. Review of theoretical descriptions pertinent to CEMS.
- V. New developments in CEMS: theory and equipment.
- VI. Potential for future developments in "surface-specific" Mössbauer spectroscopy: theory, practice, applications.

G. Ehrlich, University of Illinois at Urbana-Champaign, Illinois

An Atomic View of Crystal Growth

1. Classical Models of Growth Processes on Crystals
2. Mini-Review of Experimental Techniques with Atomic Resolution: STEM, FIM, contrast with LEED
3. Survey of Atomic Processes in Growth
  - a. Condensation
  - b. Surface Migration
  - c. Interactions with Steps
  - d. Interactions with other Adatoms and Cluster Formation
  - e. Cluster Properties and Structure
  - f. Multilayer Formation
4. Summary



T. Engel, University of Washington, Seattle, Washington

Surface Structural Determination Using Atom Diffraction

1. The atom-surface potential
  - a. Theoretical background
  - b. Experimental determination
2. Calculation of charge density contours at surfaces
3. Methods of calculating diffraction intensities
  - a. The hard wall limit
  - b. More realistic potentials
  - c. Inversion of experimental intensities to obtain charge density contours
4. Structural studies using atom diffraction
  - a. Reconstructed metal and semiconductor surfaces
  - b. Adsorption overlayers

P. J. Estrup, Brown University, Rhode Island

Reconstruction of Metal Surfaces

1. Introduction

Survey of available results for the spontaneous and adsorbate-induced reconstruction of fcc and bcc metals, obtained by LEED, HEIS and other techniques.

2. Reconstruction of W{100} and Mo{100}

- A. Structural Aspects. Review of the reversible phase transformations observed on W{100}, Mo{100}, H/W{100} and H/Mo{100}. Discussion of the phase diagrams and of the possible driving mechanism for the transitions.
- B. Chemical Consequences. Effects of reconstruction on adsorbate bonding and on desorption kinetics, studied by EELS, ESD and TDS.

3. Other Systems

Reconstruction effects in other systems, exemplified by adsorption on Pt{100}, Pd{110} and W{110}.

4. Conclusions and Summary

H. Ibach, Institut für Grenzflächenforschung und Vakuum Physik, Germany

### Surface Phonons

For two-dimensionally ordered surfaces the wave vector parallel to the surface  $q_{\parallel}$  is a good quantum number and the energies of all elementary surface excitations become a function of  $q_{\parallel}$ . In surface vibration spectroscopy so far the focus has been on the local modes of adsorbed molecules where the dispersion  $\omega(q_{\parallel})$  is small and can be neglected. Dispersion effects become important, however, for the vibrations of adsorbed molecules and the vibrational modes of the entire adsorbed molecule against the surface. Surface phonons also exist as local vibrational excitation of the substrate. It will be shown in this contribution how inelastic electron scattering may be used for mapping out the surface phonon dispersion relations on clean and adsorbate covered surfaces. In particular we have studied the clean and oxygen covered Ni{100} surface. The results will be discussed in connection with lattice dynamical models. An improved understanding of the elementary steps in the oxidation of nickel surfaces is achieved.

W. M. Gibson, State University of New York, Albany

### Ion Scattering Studies of Surface and Interface Structure

Knowledge of the atomic configuration is important to understanding chemical, electronic and mechanical processes at crystal surfaces and interfaces. During the past ten years Ion Scattering Spectroscopy (ISS) has emerged as a powerful and direct tool to get such information. Application and analysis of ion scattering divides more or less naturally into three energy regimes. Low Energy Ion Scattering (LEIS) from  $\sim 1$  to  $\sim 20$  KeV, Medium Energy Ion Scattering (MEIS) (20-200 KeV) and High Energy Ion Scattering (HEIS) (200 KeV-2 MeV). This lecture will concentrate on the physics, techniques and application of HEIS with particular attention to studies of atomic structure at interfaces - an application for which it is virtually unique.

Charged ions scatter from the screened nuclear charge of atoms of gases or solids to form a "shadow cone" behind the atom. The radius of this shadow cone is determined by the nuclear charge of the scattered ion and scattering atom and the energy of the ion and can be calculated in a straightforward way for appropriate screened coulomb atomic potentials. Atoms of a crystal may be well enough ordered that those behind the surface layers may fall within the 'shadow cone' created by atoms in the surface that they are protected from interaction with the ions in the incident beam. This may be used to get information about surface atomic structure and vibrational properties. For ions in the MeV energy range the penetration is sufficient that atomic arrangements at buried interfaces can also be probed by use of the shadow cone.

Correlated scattering from atoms along low index crystallographic rows or planes can steer and focus the incident ion beam along open "channels" in the crystal. This 'channeling' effect has been used extensively to study impurity atom positions and crystal defects inside single crystals and can also be used to get information about atomic positions at surfaces and interfaces.

Application of shadow cone and channeling phenomena to surface and interface studies will be illustrated by discussion of examples indicated on the brief outline attached after which the possibilities and limitations of the technique will be briefly discussed.

G. H. Gilmer, Bell Telephone Labs, New Jersey

#### Monte Carlo Analysis in Crystal Growth

1. Ising Models of the Crystal Surface
2. Surface Roughening of the Crystal-Vapor Interface
3. Spiral Growth
4. Impurity Mechanisms for Crystal Growth
5. Applications of the Ising Model to the Crystal-Melt Interface: Impurity Trapping in Laser-Annealed Silicon
6. Molecular Dynamics Studies of the Crystal-Vapor Interface, Surface Roughening and Surface Melting

M. Grätzel, Ecole Polytechnique Fédérale de Lausanne, Switzerland

#### Heterogeneous Photocatalysis

This paper gives an overview on photocatalytic studies involving colloidal semiconductor dispersions. Preparation and optical properties (absorption luminescence) of ultrafine (50-500 Å sized) particles of semiconducting materials such as  $\text{TiO}_2$ ,  $\text{Fe}_2\text{O}_3$  and CdS are described. Transient luminescence, absorption and conductance technique as well as time-resolved Raman spectroscopy are employed to probe interfacial electron and hole transfer to species dissolved in solution or catalysts deposited on the particles. Applications of these systems include multi-electron storage,  $\text{H}_2\text{S}$  and water cleavage by visible light.

R. Howe, University of Auckland, New Zealand

Magnetic Resonance in Surface Science

1. Introduction
2. Theoretical aspects
3. Application of EPR
  - a. identification of adsorbed radicals
  - b. transition metal ions on surfaces
  - c. surface mobility
  - d. spin echo experiments
  - e. well defined surfaces
4. Applications of NMR
  - a.  $^{29}\text{Si}$  NMR of zeolites
  - b.  $^{13}\text{C}$  NMR of adsorbed molecules
5. Summary and conclusions

R. Kelly, IBM, Watson Research Center, New York

Surface Changes by Particle Bombardment

Four groups of bombardment-induced surface alteration will be considered: structural, topographical, electronic, and compositional.

Structural changes, in which crystalline phases are converted to amorphous, amorphous phases are converted to crystalline, ordered crystalline forms are randomized, or single crystals break up into polycrystals, have been known to geologists for about a century in view of occurrence of natural amorphicity in radioactive minerals. Current interest centers on the long term storage of spent nuclear fuel, etching patterns for miniaturized electronic circuitry, and, to a lesser extent, surface analysis.

Topographical changes range from the development of facets on flat surfaces, the development of cliffs at grain boundaries, the development of ridges on mechanically damaged surfaces, to the evolution of blunt asperities into spectacular cones or pyramids. The major current interest lies in the tendency of topography, especially cones, to interfere with surface analysis. Cones may play an important role in the future as solar energy converters, as they tend to trap light.

Bombardment-induced electronic changes include the consequences of chemical changes due to the composition of the incident beam, carrier injection due to energy deposition, chemical changes due to recoil implantation, and chemical changes due to preferential sputtering. The practical aspects include easily observed, often spectacular, increases in electrical conductivity and in optical absorption.

The final aspect of bombardment-induced surface alteration occurs consequent to normal implantation, recoil implantation, and the various categories of sputtering. This is compositional change. With binary alloys the changes consist mainly in the preferential loss of the component which shows Gibbsian segregation. With oxides there are three fairly well-defined trends, according to which oxygen is lost if vapor pressures are sufficiently high or if surface binding energies are sufficiently low or if certain point-defect-based processes can occur. With halides, most examples of compositional change are explained in terms of point-defect-based processes. The practical aspects of compositional change include the synthesis of surface phases having useful chemical, electronic, or mechanical properties. More often, however, the changes are unwanted, as they interfere severely with surface analysis or with the use of sputtering to prepare crystal surfaces.

P. Kleban, University of Maine, Orono

#### Theoretical Effects of Surface Steps

(Stepped surfaces provide a means of studying influence of defects as well as finite size behavior on surface phenomena in a controlled manner. This talk will mainly be concerned with certain changes expected and observed for ordering and phase transitions on stepped surfaces.)

- I. Effects of step edge binding energy changes on overlayer ordering and LEED scattering.
- II. Surface steps and phase transitions
  1. first order transitions
    - a. theory of finite size effects
    - b. finite isotherm slopes
  2. second order transitions
    - a. finite size scaling theory
    - b. domain walls and shape effects
  3. finite size effects in systems with incommensurate order ("compression structures")

W. Mönch, Universität Duisburg, Germany

### Work Function and Band Bending at Semiconductor Surfaces

The work function of a semiconductor may be written as:

$$\Phi = E_{\text{vac}} - E_F = I + e_0 |V_s| - W_p.$$

Even if the temperature and thus  $W_p = E_F - E_{vb}$  is constant the work function may vary due to changes of the ionization energy  $I = E_{\text{vac}} - E_{vs}$  and/or the surface band bending  $e_0 |V_s| = |E_{vs} - E_{vb}|$ , i.e. due to changes of the surface dipole and the energetic distribution of surface states, respectively. We will consider in particular:

1. the temperature dependence of the work function of cleaved GaAs{110} surfaces revealing the ionization energy to be independent of temperature;
2. the influence of cleavage steps on the work function of Si{111} and GaAs{110} surfaces indicating changes of the surface dipole and in the spectrum of surface states;
3. the contribution of the reconstruction of Si{001}-2 x 1 surfaces, i.e. of the asymmetric dimers, to the work function;
4. the decrease of the work function of Si{111}, Ge{111}, and GaAs{110} surfaces by the adsorption of Cs, i.e. the formation of a dipole layer;
5. changes of the work function due to surface states created during the adsorption of Ge and the probable identification of the associated chemisorption-induced defects as  $\text{As}_{\text{Ga}}$  antisite defects.

G. A. Somorjai, University of California, Berkeley

### The Surface Science of Heterogeneous Catalysis

Modern surface science during the past 15 years developed a large number of techniques that can be utilized to uncover the molecular ingredients of heterogeneous catalysis. The atomic surface structure, the chemical bonding of adsorbates, the composition and oxidation states of surface atoms can all be determined within the sensitivity of less than 1% of a monolayer (about  $10^{13}$  atoms per  $\text{cm}^2$ ).

Catalysis is a kinetic phenomenon; reactant molecules adsorb, rearrange and desorb from the surface continuously. It is generally carried out at high pressures (atmospheres) and the kinetic parameters, rate, activation energy and the product distribution reflect the activity and the selectivity of the catalysts to obtain the desired products. In order to unravel the molecular ingredients of heterogeneous catalysis, we had to combine catalytic reaction rate studies that were carried out at high pressures (several atmospheres) with surface analysis of the catalyst surface that usually required ultra high vacuum conditions. We therefore developed techniques that permitted us to do both in the same instrument. In the low-pressure-high-pressure apparatus a small area sample was placed in the center of an ultrahigh vacuum chamber. For the high pressure phase of the study, a small cup with a total volume of  $50 \text{ cm}^3$  could be placed over the crystal sample to isolate it from the rest of the chamber. This isolation cell could be pressurized to over 100 atmospheres, as required, using a mixture of gaseous reactants, thus providing a small, high-pressure reaction chamber. This was connected to a gas chromatograph that monitored both rate and product distributions. The structure and composition of the surface can be determined by electron scattering before and after the high pressure experiments by removal of the cup. The crystal sample could be heated during both low and high pressure experiments. Our samples are single crystals or polycrystalline foils of about one  $\text{cm}^2$  surface area. Such small area catalysts are entirely adequate for surface analysis as well as for detecting the product distributions and the rates obtained during catalytic reaction studies.

The small area single crystals are model catalysts. Models are used frequently in physical sciences to uncover the working of a complex system. Of course, it must be ascertained that the model system behaves similarly to that of the more complex chemical system that is to be ultimately utilized. The model small area catalysts were compared with dispersed high surface area catalysts in the same reaction under identical experimental conditions. The same turnover rates, product distributions and activation energies were obtained for the ring opening of cyclopropane and the hydrogenation of benzene over platinum and for carbon monoxide hydrogenation over rhodium. It appears that for catalyzed reactions that do not exhibit much structure sensitivity, small area crystal and large are dispersed particles of the same metal yield identical catalytic reaction parameters.

We have concentrated our studies of molecular scale catalysis on transition metals which catalyze hydrocarbon conversion reactions and on the hydrogenation of carbon monoxide. Platinum, an excellent catalyst for dehydrocyclization reactions that produce aromatic molecules from alkanes, or for isomerization, was one of the metals we studied intensively. The other was rhodium, which was found to produce oxygenated organic molecules from carbon monoxide and hydrogen, selectively. Iron that catalyzes ammonia synthesis from nitrogen and hydrogen as well as the  $\text{CO}/\text{H}_2$  reaction and was also a focus of our investigations. We investigated in detail the photodissociation of water over oxide surfaces and the hydrogenation of graphite to methane; both reactions are catalyzed by alkali metal ions. Out of these studies came the identification of three necessary ingredients of selective molecular scale catalysis.

- 1) Atomic surface structure
- 2) An active carbonaceous deposit
- 3) The proper oxidation state of surface atoms

We shall review each of these reaction parameters in order to understand how the catalytic reactions occur after describing some of the important concepts of heterogeneous catalysis.

J. Stöhr, Exxon Research and Engineering Co., New Jersey

#### Surface Crystallography by Means of NEXAFS and SEXAFS

The availability of high brightness (flux/unit area) monochromatized synchrotron radiation allows the application of the extended x-ray absorption fine structure (EXAFS) and near edge x-ray absorption fine structure (NEXAFS) techniques to the study of the crystallographic structure of surfaces. Surface EXAFS (SEXAFS) studies were first performed in 1978 and since then the SEXAFS technique has been developed into a reliable and accurate surface structural tool. The NEXAFS technique was also used for the first time during the late 1970's and has been applied successfully to study the structural arrangement of chemisorbed atoms and molecules. Both NEXAFS and SEXAFS studies measure the absorption coefficient of a surface atom and are typically carried out by detection of the electron yield (Auger yield or total electron yield) signal from the surface as the photon energy is swept through the absorption edge of a chemisorbed atom or molecule. In certain cases it is also possible to obtain NEXAFS and EXAFS spectra by monitoring the photon stimulated desorption of ions from the surface. For a review of the principles, analysis and applications of SEXAFS the reader is referred to other references.

SEXAFS studies monitor the oscillatory structure above the K or L absorption edge of a surface atom. The bond distances from the central absorbing atom to its neighbors on the surface are determined from analysis of the phase of the sinusoidal EXAFS oscillations by comparison with a model compound of known structure. Because only the EXAFS oscillations are analyzed which correspond to the scattering of energetic photoelectrons (kinetic energy > 50 eV) the scattering is dominated by the core electron potentials of the absorbing (central) and backscattering (neighbor) atoms. Therefore, the scattering phaseshift is the same for the same atom pair in chemically different compounds and can be transferred. The coordination number (or chemisorption site) is obtained from the amplitude of the SEXAFS signal. The absolute coordination number is deducted by amplitude comparison of the surface system with a model compound. In order to determine the chemisorption site on a single crystal surface it is usually sufficient to measure the polarization dependence (turning the sample in the polarized x-ray beam) of the SEXAFS amplitude or to determine the second nearest



neighbor distance. Since x-ray absorption is a local process and a given atom can be selected by its absorption edge SEXAFS can be applied to ordered as well as disordered (e.g. amorphous) surfaces. Applications of the technique in the past have ranged from chemisorption phenomena to the study of solid-solid interface formation. The most important reason for the success of SEXAFS lies in the simple theoretical interpretation of the EXAFS process which allows a straightforward determination of the basic structural parameters without the necessity of theoretical calculations.

NEXAFS studies focus on the fine structure close to the absorption edge. This energy region extending out to about 50 eV past the edge is typically not considered in the EXAFS analysis because of the importance of multiple-scattering effects which also dominate in low energy electron diffraction (LEED). However, although more difficult to interpret this region contains rich and sizeable absorption structure which because of the intrinsic anisotropy of surfaces usually exhibits a dramatic polarization dependence. The most pronounced near edge effects are observed for chemisorbed molecules. Here the NEXAFS is dominated by intra-molecular excitations with surprisingly little influence from scattering contributions due to surface substrate atoms. In most cases giant resonances are observed which arise from transitions of a core electron to empty or partially filled molecular final states (bound state resonances) and/or to continuum final states with an enhanced amplitude on the molecule (shape resonances). These transitions are governed by dipole selection rules and symmetry considerations allow the precise determination of the molecular orientation on the surface. In the future it should be possible to also determine the structural arrangement of chemisorbed atoms by comparison of experimental NEXAFS spectra and multiple scattering calculations of the near edge absorption.

J. H. van der Merwe, University of Pretoria, Republic of South Africa

#### Recent Developments in the Theory of Epitaxy

This lecture is tailored towards the fundamental understanding of epitaxy, rather than practical applications, but will have its evident contributions to the latter. Although aimed at recent developments, clarity requires that facts which have been known for many years, be briefly recalled. Also, the early stages of growth are, in certain cases, significant in shaping the intermediate and final epitaxial orientations and structures. These stages will be briefly dealt with in the context of epitaxy. The lecture will contain descriptions (i) of important observations; e.g. on growth morphology, misfit accommodation, overlayer mobility and interface alloying, (ii) of the relevant parameters, such as misfit and bonding and governing principles for equilibrium and non-equilibrium configurations, (iii) of the models and simplifications needed in the theory, (iv) of the application of the model in predicting epitaxial orientations and (v) of structural, orientational and compositional changes during growth. Speculations on needs and future trends will be presented.

N. Winograd, Pennsylvania State University, University Park

### Angle-Resolved SIMS

- I. Introduction to ion beam/solid interactions
  - A. Theoretical models for the momentum dissipation
  - B. Angular distributions of atoms ejected from clean single crystals
  - C. Theory of the molecular cluster formation process
- II. Angle-resolved SIMS for atomic overlayers on single crystals
  - A. O/Cu{100}
  - B. O/Rh{111}
- III. Orientational studies of adsorbed molecules by angle-resolved SIMS of ejected molecular cluster species
  - A.  $\text{Ni}_2^+$  from Ni{100}
  - B.  $\text{NiCO}^+$  from C(2x2) CO-Ni{100}
  - C.  $\text{NiCO}^+$  from the CO-Ni{7 9 11} stepped surface
  - D.  $\text{AgC}_6\text{H}_6^+$  and  $\text{AgC}_5\text{H}_6^+$  from Ag{111}
- IV. Prospects for angle-resolved analysis of ejected neutrals by multiphoton resonance ionization

M.J. Yacaman, Universidad Nacional Autonoma de Mexico, Mexico

### Structure Determination of Small Catalytic Particles by Electron Microscopy

1. Electron diffraction of individual particles in the range 10 - 500 Å
  - a) Structure determination - Examples of FCC and non-FCC particles
  - b) Morphological information on diffraction patterns. Fine structure of diffraction spots and its relation with the particle shape
  - c) Defects on particles and its effect on diffraction spots
  - d) Simulation of diffraction patterns of small particles

2. Weak-beam dark field and atom resolution of small particles
  - a) Examples of shape determination using weak-beam images and its correlation with structure
  - b) Images of defects in small particles
  - c) Atom resolution images in small metallic particles
3. Techniques for studying supported particles
  - Topographic images of the catalyst support
  - Images of 5 Å particles using refraction methods
  - Studies of Epitaxial relationships
4. Surface reconstruction in thin films and metal particles
  - Diffraction methods to study surface reconstruction in the electron microscope
  - Surface reconstruction in thin metal films and corresponding dark field images
  - Surface reconstruction in small particles

Since the discussions are an essential part of ISISS, the Session Chairmen play an important role. At ISISS 1983, the following surface scientists served as Chairmen:

Dr. V. Haensel  
University of Massachusetts  
Department of Chemical Engineering  
Amherst, MA 01003

Professor W. Keith Hall  
University of Wisconsin-Milwaukee  
Dept. of Chemistry  
Milwaukee, WI 53201

Dr. H. Skala  
Universal Oil Products, Inc.  
Corporate Research Center  
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Professor George W. Keulks  
University of Wisconsin-Milwaukee  
Department of Chemistry  
Milwaukee, WI 53201

Dr. D. Gruen  
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9700 South Cass Avenue  
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Professor M. Steinberg  
The Hebrew University of Jerusalem  
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Professor Max Legally  
University of Wisconsin-Madison  
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Madison, WI 53706

Professor R. Gomer  
University of Chicago  
James Franck Institute  
Chicago, IL 60637

Professor S. Y. Tong  
University of Wisconsin-Milwaukee  
Department of Physics  
Milwaukee, WI 53201

One hundred and sixty-two scientists from all parts of the U.S.A., from Germany, Israel, Japan, Mexico, New Zealand, People's Republic of China, South Africa, Switzerland, and Viet Nam participated. They came from universities (75%), from industry (21%), as well as government institutions (4%). The educational value of the conference is demonstrated by the fact that about 42% of the participants were Graduate Students and Post-Doctoral Fellows. The registration fee was kept as low as possible.

The following registration fees were requested:

Registration before July 22, 1983:

\$75.00 Regular  
\$37.00 Graduate Students and Post-Doctoral Fellows

Registration after July 22, 1983:

\$95.00 Regular  
\$47.00 Graduate Students and Post-Doctoral Fellows

Students in the UW-System paid a nominal fee.

Besides the scientific program, a number of social programs were arranged. They included dinner tours, a reception for speakers and participants from foreign countries, and a banquet. Many participants used the opportunity to visit the facilities of the Laboratory for Surface Studies at UWM. In connection with the Summer Institute, an exhibition of surface science books was organized.

International scientific societies and journals announced the conference. About 2700 scientists were contacted directly.

As in the case of former ISISS, the lecturers also wrote review papers which are published collectively in form of a single volume book. Volume V of "Chemistry and Physics of Solid Surfaces" is printed by Springer Verlag, Berlin-Heidelberg-New York.

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Dr. Ralf Vanselow  
Director of ISISS

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